

Advanced Statistical Physics

TD1 Ergodicity & baths

September 2022

1 Ergodicity

Figure 1 (a) shows one time series of a stochastic process, $X(i)$, $i = 1, \dots, n$, in other words, an indexed set of random variables in which the integer i represents a discrete time. Panel (b) is the histogram of $X(i)$ with $i = 1, \dots, 100$ over one time series. Panel (c), the histogram of X at a particular instant $i = 25$ measured using $N = 100$ different realisations of the stochastic process.

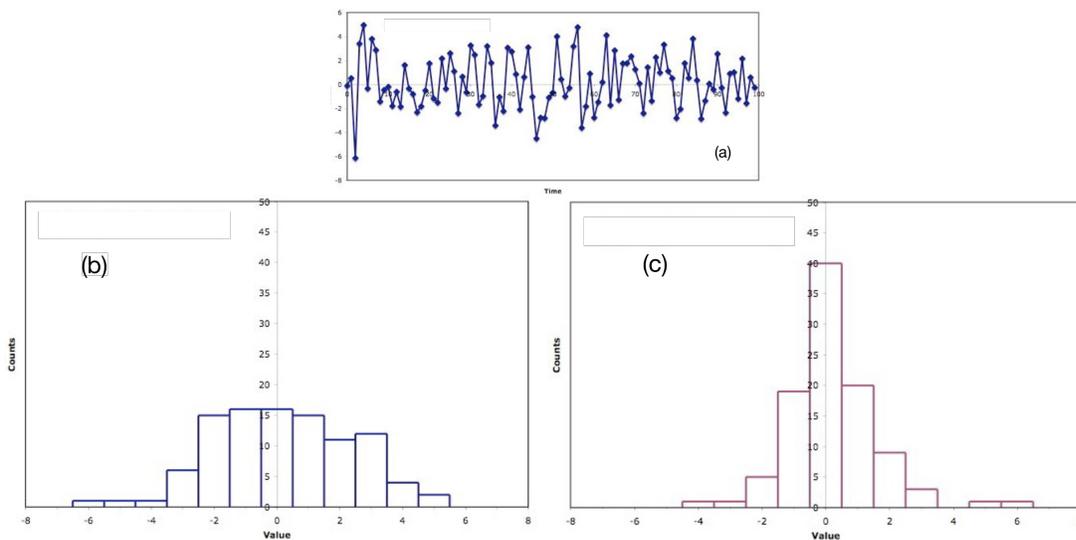


FIG. 1 – (a) A time series of the stochastic process $X(i)$, with $i = 1, \dots, 100$. (b) The histogram of $X(i)$ with $i = 1, \dots, 100$ over one time series. (c) The histogram of $X_a(i = 25)$ over $a = 1, \dots, N = 100$ realizations of the stochastic process.

1. In your opinion, is this process ergodic? Give the condition needed to satisfy ergodicity. Explain your conclusion concerning this process. Give a general argument without an explicit calculation and then justify it with a calculation.
2. Which kind of improved measurement(s) would you propose to reach a more certain answer to the previous question?

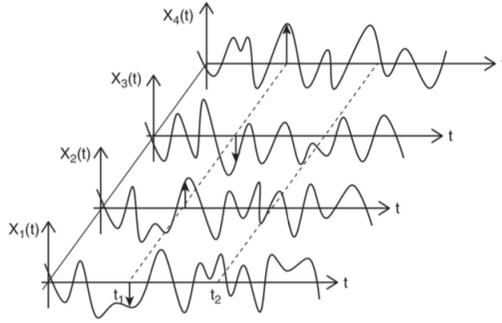


FIG. 2 – Four realisations of a continuous time stochastic process.

Four signals (realisations) of another continuous time random process X are displayed in Fig. 2. Is this process ergodic?

2 Coupling to environments and irreversibility

Consider now, for simplicity a single particle with mass M and potential energy $V(x)$, confined to move in one dimension, and imagine that it is itself bi-linearly coupled to an ensemble of harmonic oscillators which, to further ease the calculations we will take in their “diagonalised” formulation. The coupled system represents a system (the particle) and an environment (the ensemble of oscillators). The interacting system+environment ensemble is ‘closed’ while the system is ‘open’. The nature of the environment, *e.g.* whether it can be modeled by a classical or a quantum formalism, depends on the problem under study. We focus here on the classical problem defined by H_{tot} :

$$H_{\text{tot}} = H_{\text{syst}} + H_{\text{env}} + H_{\text{int}} + H_{\text{counter}} = H_{\text{syst}} + \tilde{H}_{\text{env}} . \quad (1)$$

H_{syst} is the Hamiltonian of the isolated particle,

$$H_{\text{syst}} = \frac{p^2}{2M} + V(x) , \quad (2)$$

with p and x its momentum and position. H_{env} is the Hamiltonian of a ‘thermal bath’ that, for simplicity, we take to be an ensemble of N independent harmonic oscillators with masses m_a and frequencies ω_a , $a = 1, \dots, N$

$$H_{\text{env}} = \sum_{a=1}^N \frac{\pi_a^2}{2m_a} + \frac{m_a \omega_a^2}{2} q_a^2 \quad (3)$$

with π_a and q_a their momenta and positions. H_{int} is the coupling between system and environment. We will restrict the discussion to a linear interaction in the oscillator coordinates, q_a , and in the particle coordinate,

$$H_{\text{int}} = x \sum_{a=1}^N c_a q_a , \quad (4)$$

with c_a the coupling constants. The counter-term H_{counter} is added to avoid the generation of a negative harmonic potential on the particle due to the coupling to the oscillators (that may render the dynamics unstable).

A derivation of a generalized Langevin equation with memory is very simple starting from Newton dynamics of the full system. The generalization to more complex systems and/or to more complicated baths and higher dimensions is straightforward.

1. Write Hamilton's equations for the particle.
2. Write Hamilton's equations for the oscillators in the bath.
3. Solve the latter and introduce the solution in the former.
4. Write the resulting equation as

$$\dot{p}(t) = -V'[x(t)] + \xi(t) - \int_0^t dt' \Gamma(t-t')\dot{x}(t') \quad (5)$$

and identify the symmetric and stationary kernel Γ and the time-dependent force ξ .

This is the equation of motion of the reduced system. It is still deterministic. $\xi(t)$ is a sum of oscillating functions of time. The third term on the rhs of eq. (5) represents a rather complicated friction force. Its value at time t depends explicitly on the history of the particle at times $0 \leq t' \leq t$ and makes the equation non-Markovian. One can rewrite it as an integral running up to a total time $\mathcal{T} > \max(t, t')$ introducing the retarded friction:

$$\gamma(t-t') = \Gamma(t-t')\theta(t-t'). \quad (6)$$

Until this point the dynamics of the system remain deterministic and are completely determined by its initial conditions as well as those of the reservoir variables. Two important points can be made here. On the one hand, one can check, by simple numerical generation, that the function ξ at, say, fixed t resembles more and more a random variable as the number of oscillators increases (for incommensurate frequencies ω_a). The initial conditions for the oscillators are the seeds of the random number generator. This is similar to what happens with random number generators in the sense that these are, ultimately, periodic functions with a finite recurrence time that, however, can be made sufficiently long for computational purposes. Therefore, ξ is a pseudo random number. On the other hand, one can directly introduce the statistical element into play when one realises that it is impossible to know the initial configuration of the large number of oscillators with great precision and one proposes that the initial coordinates and momenta of the oscillators have a canonical distribution at an inverse temperature β . (Note that one needs to assume that the oscillators interacted in the past to establish ergodicity and reach this pdf, though they do not do any longer.) Then, one chooses $\{\pi_a(0), q_a(0)\}$ to be initially distributed according to a canonical phase space distribution:

$$P(\{\pi_a(0), q_a(0)\}, x(0)) = 1/\tilde{\mathcal{Z}}_{\text{env}}[x(0)] e^{-\beta\tilde{H}_{\text{env}}[\{\pi_a(0), q_a(0)\}, x(0)]} \quad (7)$$

with $\tilde{H}_{\text{env}} = H_{\text{env}} + H_{\text{int}} + H_{\text{counter}}$, that can be rewritten as

$$\tilde{H}_{\text{env}} = \sum_{a=1}^N \left[\frac{m_a \omega_a^2}{2} \left(q_a(0) + \frac{c_a}{m_a \omega_a^2} x(0) \right)^2 + \frac{\pi_a^2(0)}{2m_a} \right]. \quad (8)$$

Again, the presence of H_{counter} here is for convenience. The randomness in the initial conditions gives rise to a random force acting on the reduced system.

1. Prove that ξ is a Gaussian random variable, that is to say a noise, with

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = k_B T \Gamma(t-t'). \quad (9)$$

(One can easily check that higher-order correlations vanish for an odd number of ξ factors and factorise as products of two time correlations for an even number of ξ factors.) In consequence ξ has Gaussian statistics.

2. Defining the inverse of Γ over the interval $[0, t]$, $\int_0^t dt'' \Gamma(t-t'')\Gamma^{-1}(t''-t') = \delta(t-t')$, confirm that one has the Gaussian pdf:

$$P[\xi] = \mathcal{Z}^{-1} e^{-\frac{1}{2k_B T} \int_0^t dt \int_0^t dt' \xi(t)\Gamma^{-1}(t-t')\xi(t')}. \quad (10)$$

\mathcal{Z} is the normalisation. A random force with non-vanishing correlations on a finite support is usually called a coloured noise. Equation (5) is now a genuine Langevin equation.

3. A multiplicative retarded noise arises from a model in which one couples the coordinates of the oscillators to a generic function of the coordinates of the system. Prove that for a non-linear coupling $H_{\text{int}} = \mathcal{V}[x] \sum_{a=1}^N c_a q_a$ there is a choice of counter-term for which the Langevin equation reads

$$\dot{p}(t) = -V'[x(t)] + \xi(t)\mathcal{V}'[x(t)] - \mathcal{V}'[x(t)] \int_0^t dt' \Gamma(t-t')\mathcal{V}'[x(t')]\dot{x}(t')$$

with the same Γ and $\xi(t)$. The noise appears now multiplying a function of the particles' coordinate. Applications of this kind of equations are manifold. For instance, the random motion of a colloid in a confined medium is mimicked with a Langevin equation in which the friction coefficient depends on the position notably close to the walls.

3 Extra

Take a one dimensional mono-atomic material and denote the position of each atom x_n , with $n = 1, \dots, N$. In equilibrium, the atoms sit at regular positions $x_n = na$ with a the lattice spacing. One assumes that only the interactions between adjacent atoms are important and that the two-body potential that holds the atoms in place takes the form $\sum_n V(x_n - x_{n-1})$. For small deviations from equilibrium, one can expand the generic V to second order in the displacements

$$u_n = x_n - na \quad (11)$$

and the potential becomes the one of a set of coupled harmonic Hooke oscillators. The Hamiltonian governing the dynamics is then

$$H = \sum_n \frac{p_n^2}{2m} + \frac{\kappa}{2} \sum_n (u_n - u_{n-1})^2, \quad (12)$$

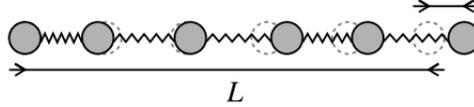


FIG. 3 – A chain of identical masses connected by massless springs. The dotted disks represent the regular equilibrium positions while the solid ones the actual positions during motion. The displacement of the disk at the right boundary from its equilibrium position is indicated above it. The length of the chain is $L = aN$.

where $p_n = m\dot{u}_n$ and m and κ are material parameters. The Hamiltonian is the one of a chain of identical masses connected by identical massless springs with spring constant κ as the one depicted in Fig. 3.

1. Write Newton's equations of motion.
2. To ease the solution of these equations we impose periodic boundary conditions, extending $n \in \mathbb{Z}$ and requiring $u_{n+N} = u_n$. This choice does not influence the physical behaviour for $N \gg 1$. Show that the real (or imaginary) parts of the plane waves

$$u_n = Ae^{-i\omega t - ikna} \quad (13)$$

solve the equations of motion.

3. Using the fact that u_n in eq. (13) is invariant under $k \mapsto k + 2\pi/a$ restrict k to lie in the first Brillouin zone $k \in [-\pi/a, \pi/a)$. Find the quantisation condition on k assuming, for simplicity, that N is even.
4. Evaluate the effect of a and aN on the behaviour of the wave-vector k .
5. Find the *dispersion relation*, that is to say, the relation between ω and k .
6. Plot this relation. What is the behaviour for $k \simeq 0$?
7. Calculate the phase velocity $v_p = \omega(k)/k$ and the group velocity $v_g = d\omega(k)/dk$. v_p is the velocity of the propagation of the plane wave, whereas v_g is the velocity of the propagation of the wave packet. The latter is the velocity for the propagation of energy in the medium. At low k , $v_p = v_g$ and represent the speed of sound of the material.
8. What is the energy of a mode k ?
9. In the limit $k \simeq 0$?
10. What is the density of states in the limit $L \rightarrow \infty$? To make calculations simple we will focus on low energy values $E \simeq 0$.

The dispersion relation found with this model is in very good qualitative agreement with the ones measured in real crystals.

This model is used in the Altland & Simons textbook to introduce an effective field theory for the low-energy excitations. We will see this kind of construction in the Lectures. They also point out, as usually done, that this very simple problem gives already sufficient

information to justify the need to consider quantum fluctuations. see the graph in the right in Fig. 4.

Although the exercise focused on the one-dimensional lattice, the same basic characterisation of phonon branches occurs for higher dimensional lattices. The time-dependent displacement of an atom identified by the indices of its equilibrium position \mathbf{r}_n , on a d dimensional regular *Bravais* lattice in which there is one atom per unit cell, is

$$\mathbf{u}_n(t) = \boldsymbol{\varepsilon}_n e^{i\omega(\mathbf{k})t + i\mathbf{k}\cdot\mathbf{n}a} \quad (14)$$

The wave vector \mathbf{k} specifies both the wavelength and direction of propagation. The vector $\boldsymbol{\varepsilon}_n$ determines the amplitude as well as the direction of vibration of the atoms. Thus, this vector specifies the *polarization* of the wave, i.e., whether the wave is *longitudinal* ($\boldsymbol{\varepsilon}_n$ parallel to \mathbf{k}) or *transverse* ($\boldsymbol{\varepsilon}_n$ perpendicular to \mathbf{k}). Replacing (14) in the equations of motion one finds d equations that impose d different conditions on $\omega(\mathbf{k})$ and give rise to three acoustic branches, all with linear dispersion $\omega \sim |\mathbf{k}|$ for low momenta, while optical branches have non-vanishing frequency, typically higher than the acoustic branch.

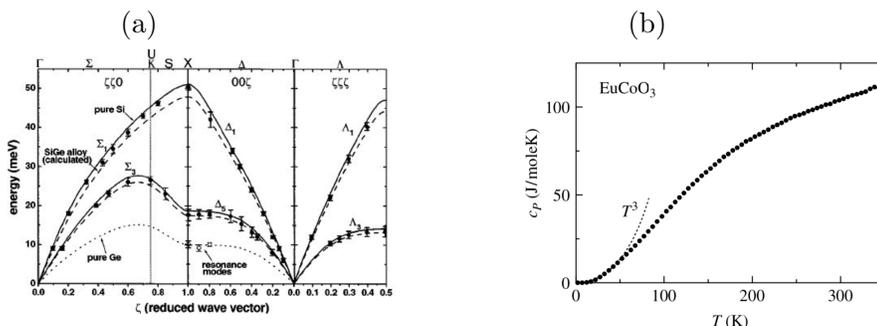


FIG. 4 – (a) Dispersion relation of acoustic phonons in the $\text{Si}_{0.92}\text{Ge}_{0.08}$ alloy. Figure from D. Le Bolloc'h, J. L. Robertson, H. Reichert, S. C. Moss, and M. L. Crow, *X-ray and neutron scattering study of Si-rich Si-Ge single crystals*, *Phys. Rev. B* **63**, 035204 (2001). (b) Specific heat of EuCoO_3 . Figure taken from the Altland & Simons textbook. At high T the curve approaches a constant, as predicted by the classical harmonic model (equipartition) but at low T there is a clear variation of the curve which indicates the need to take quantum fluctuations into account.

As further exercise of similar kind, study the di-atomic harmonic chain, in which atoms of two different masses, m and M , intercalate on the chain. Show that a second dispersion relation gives rise to an additional branch, the optical one.

A. Altland and B. Simons, *Condensed Matter Field Theory* (Cambridge University Press).